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6. AUTHOR(S)

Dr Rodney J. Bartlett

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Dept of Chemistry & Physics
University of Florida
P.O. Box 118435
Gainesville FL 32611-8435

8. PERFORMING ORGANIZATION REPORT NUMBER

9 SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

AFOSR/NL
110 Duncan Ave Room B115
Bolling AFB DC 20332-8050

Dr Michael R. Berman

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13 ABSTRACT (Maximum 200 words)

The Coupled Cluster Theory Electron Correlation Workshop "Fifty Years of the Correlation Problem" was held at Cedar Key, Florida, from June 15-19, 1997, to recognize the essential developments for one of the dominant topics in the quantum theory of atoms, molecules, and solids. The instantaneous Coloumbic interactions among electrons that correlate their motion (the electron correlation problem) has been the focal point of ab initio quantum chemistry and physics for many years. Only with the proper inclsion of electron correlation in approximate solutions of the Schroedinger (or Dirac-Fock) equation is it possible to provide predictive accuracy for most properties of atoms and molecules. Such quantities include energetics (involving multiplets, dissociation pathways, and activation barriers), excited states and first- and second-order properties (like moments, field, gradients, polarizabilities, and magnetic susceptibilities), and vibrational, electronic, EPR and NMR spectra, among others.

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THE COUPLED CLUSTER THEORY ELECTRON CORRELATION WORKSHOP "FIFTY YEARS OF THE CORRELATION PROBLEM"

The Coupled Cluster Theory Electron Correlation Workshop "Fifty Years of the Correlation Problem" was held at Cedar Key, Florida, from June 15-19, 1997, to recognize the essential developments for one of the dominant topics in the quantum theory of atoms, molecules, and solids. The instantaneous Coloumbic interactions among electrons that correlate their motion (the electron correlation problem) has been the focal point of *ab initio* quantum chemistry and physics for many years. Only with the proper inclusion of electron correlation in approximate solutions of the Schroedinger (or Dirac-Fock) equation is it possible to provide predictive accuracy for most properties of atoms and molecules. Such quantities include energetics (involving multiplets, dissociation pathways, and activation barriers), excited states and first- and second-order properties (like moments, field, gradients, polarizabilities, and magnetic susceptibilities), and vibrational, electronic, EPR and NMR spectra, among others.

In extended systems like polymers and solids, correlation effects are critical to properties like cohesive energies, energy bands, and particularly band gaps; other optical properties like exciton spectra or non-linear optical behavior; and collective phenomena as in conductivity and superconductivity. Without adequate inclusion of electron correlation, theory cannot be predictive.

About 50 years after the correlation problem was clearly identified, we were in a position to report on the remarkable progress that has been made and to point the way to the future. These accomplishments have been achieved by a combination of critical formal and methodological developments in the theory such as coupled-cluster theory, many-body perturbation theory, propagator methods, and of configuration interaction methods coupled to the dramatic progress in computational power. Together, today, accurate applications to molecular many-electron systems are possible. This meeting addressed developing a similar capability for the reliable introduction of electron correlation to extended systems.

To achieve some historical perspective, several of the pioneer investigators who have made contributions to the correlation problem spoke at the meeting. This, in fact, enabled us to have representatives of the four scientific generations of investigators who have worked on the correlation problem.

The meeting was attended by 88 scientists from over 30 different countries. Thirty-seven invited presentations were made, augmented by 37 poster presentations. In a panel session, we addressed the timely topic of "With Density Functional Theory, Is there Any Future for *ab initio* Correlated Methods?" which generated much discussion.

The Proceedings, which consists of 25 papers, will be published in *Molecular Physics.* Copies of the Proceedings will be sent to AFOSR as instructed when they become available.